BIOTECHNOLOGY

UDC 602.4:66.06
DOI: 10.18372/2306-1472.74.12298

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FEATURES OF THE MATERIAL BALANCE CALCULATION OF THREE-PHASE MIXTURES FOR EXTRACTION PROCESSES

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Abstract

Purpose: *improvement of the algorithm for calculating the liquid-liquid-vapor equilibria for binary and ternary mixtures (in application for extraction processes).* ***Methods:*** *analysis of phase diagrams, modeling of cutting off a part of an equilibrium phase, algebraic transformations of the system of Eqs. describing a single-step evaporation of a three-phase mixture of a given composition.* ***Results:*** *for two types of phase diagrams of binary mixtures with partial miscibility of components in the liquid phase, restrictions on the possible values of the mole fractions of the vapor and two liquid phases under the equilibrium conditions of the liquid-liquid-vapor mixture for a given total composition were obtained. For ternary mixtures, analytical expressions for the calculation of three phases composition for the given two sets of distribution coefficients were obtained. Formulas for calculating mole fractions of vapor and two liquid phases according to the given composition of the mixture are obtained. The following formulas are used to calculate the three-phase equilibrium of the butylene-n-butane-water mixture based on the Raoult's and Henry's Laws.* ***Discussion:*** *the obtained formulas can be used to determine approximately the composition of coexisting equilibrium phases of ternary mixtures as well as the mole fractions of phases. For binary mixtures, it is expedient to supplement the input information of the single-step evaporation of a mixture of a given composition with the permissible value of the mole fraction of the vapor phase.*

Keywords: biotechnology; extraction; liquid-liquid-vapour equilibrium; K-value; mixture; calculation; material balance.

1. Introduction

Liquid-liquid extraction processes are widely used in biotechnological industries [1 - 3]. Usually there is a vapor phase, therefore, three-phase liquid-liquid-steam systems should be considered more strictly. The necessary part of the calculation of an extraction process is the solution of the problem of isobaric-isothermal evaporation of a three-phase mixture of a given overall mixture composition.

2. Analysis of the latest research and publications

One of the common approaches to the formulation of this problem for a n-component mixture (where n is the number of components) involves the solution of the following system of Eqs. [4-7]:

- Eqs. of the material balance, which reflect the conditions of the closed system:

$$z_i = y_i \cdot V + x_{1i} \cdot L_1 + x_{2i} \cdot L_2 \qquad (1)$$

- Eqs. that reflect the requirement that the mole fractions sum to unity in each phase:

$$\sum_{i=1}^{n} y_i = 1,\ \sum_{i=1}^{n} x_{1i} = 1, \sum_{i=1}^{n} x_{2i} = 1 \qquad (2)$$

and equation of normalization of mole fractions of the phases:

$$V + L_1 + L_2 = 1 \qquad (3)$$

where z_i, y_i, x_{1i}, x_{2i}, are the mole fractions of the i-th component in the mixture, the vapor phase, the first (more volatile) liquid phase L1, second liquid phase L2, respectively; V, L_1, L_2 are the mole fractions of the phases in equilibrium.

For the solution of Eqs. (1-3), distribution coefficients for the components distributed between the vapor and the corresponding liquid phase are usually used:

$$K_{1i} = \frac{y_i}{x_{1i}},\ K_{2i} = \frac{y_i}{x_{2i}} \qquad (4)$$

which makes it possible to reduce the system of Eqs. (1-4) to the system of two nonlinear Eqs. with two unknowns [4]:

$$\begin{cases} \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} x_{1i} = \sum_{i=1}^{n} a_i \cdot A_i = 0 \\ \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} x_{2i} = \sum_{i=1}^{n} b_i \cdot A_i = 0 \end{cases} \qquad (5)$$

where $A_i = \dfrac{z_i}{V + \dfrac{(1-V)C}{K_{1i}} + \dfrac{(1-V)(1-C)}{K_{2i}}}$,

$a_i = 1 - \dfrac{1}{K_{1i}}$, $b_i = 1 - \dfrac{1}{K_{2i}}$, $C = \dfrac{L_1}{L_1 + L_2}$.

For the system of Eqs. (5), the given values are z_i, K_{1i} and K_{2i}, while V, C must be determined.

When solving systems of nonlinear Eqs. certain difficulties may arise, which sometimes leads to failures of the calculation algorithm. The general algorithm also does not take into account the features of binary and ternary mixtures.

3. Research tasks

The aim of the study is to analyze the features of the solution of Eqs. (1-5) for binary and ternary mixtures.

4. Research methods

To analyze the properties of binary and ternary three-phase mixtures, we apply the Gibbs' phase rule, consider the form of typical phase diagrams, simulate the isobaric-isothermal fragmentation of the equilibrium phase while maintaining the three-phase equilibrium, consider the typical experimental data on the equilibrium of liquid-liquid-vapor, and the constraints embedded in the Eqs. (1-4).

5. Results

In accordance with the Gibbs phase rule, a binary three-phase mixture is a univariant system. Given one intensive variable (temperature or pressure), all other intensive variables are uniquely fixed. This thermodynamic feature is transformed into a mathematical singularity of the system of Eqs. (5). For n = 2, the Eqs. (5) are linearly bounded by the relation: $\dfrac{a_1}{a_2} = \dfrac{b_1}{b_2}$. This ratio is easy to obtain, if we apply the method of the sequential exclusion of unknowns to the system of Eqs. (1-4). The ratio can be written as:

$$(1 - \frac{1}{K_{11}})(1 - \frac{1}{K_{22}}) = (1 - \frac{1}{K_{12}})(1 - \frac{1}{K_{21}}) \qquad (6)$$

That is, only three out of four distribution coefficients, which are defined to describe the liquid-liquid-vapor equilibrium, are independent. This feature should be taken into account when choosing and applying models for the definition of K_{ij}.

Let's show that for two-component systems there are certain restrictions on possible relationships of mole fractions of equilibrium phases for a given overall composition of the mixture. The analytical form of these restrictions depends on the relationship between the values y_1, x_{11} and x_{21}.

Fig. 1 and 2 show phase diagrams for heteroazeotropic and zeotropic mixtures.

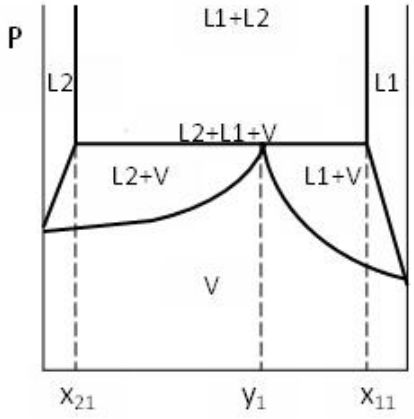
For the more volatile component of a heteroazotropic mixture (e.g., water (1) - ethylbenzene (2) [8]) $x_{11} > y_1 > x_{21}$. With isobaric-isothermal expansion of a three-phase mixture of an invariant overall composition z_1 (provided $y_1 \geq z_1 \geq x_{21}$) there is evaporation of both liquid phases, but the more volatile liquid phase 1

disappears first (Fig. 3 a), and the limit value under conditions of three-phase equilibrium is L_1=0. If we substitute L_1 = 0 into Eqs. (1, 3), then under this condition we obtain the minimum value of the second liquid phase L_2 and the maximum value of the vapor phase V. At isobaric-isothermal compression of the three-phase mixture at all values $x_{11} \geq z_1 \geq x_{21}$ the vapor phase disappears, (Fig. 3 c), and the limit value for the three-phase equilibrium is V=0. Let's substitute V = 0 into Eqs. (1, 3) and get the maximum values of L_{1max} and L_{2max}.

Provided $y_1 \geq z_1 \geq x_{21}$, we get the following restrictions:

$$0 \leq V \leq \frac{z_1 - x_{21}}{y_1 - x_{21}}, \qquad 0 \leq L_1 \leq \frac{z_1 - x_{21}}{x_{11} - x_{21}},$$

$$\frac{y_1 - z_1}{y_1 - x_{21}} \leq L_2 \leq \frac{x_{11} - z_1}{x_{11} - x_{21}} \qquad (7)$$



. Fig. 1. Pressure-composition phase diagram (at constant temperature) for heteroazeotropic binary system having partially miscible liquid phases

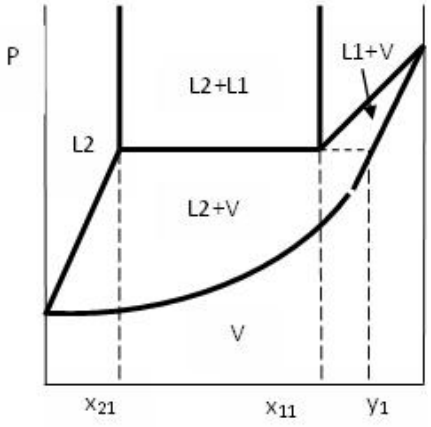


Fig. 2. Pressure-composition phase diagram (at constant temperature) for zeotropic binary system having partially miscible liquid phases

Provided $x_{11} \geq z_1 \geq y_1$, the less volatile phase 2 disappears at expansion. Respectively:

$$0 \leq V \leq \frac{x_{11} - z_1}{x_{11} - y_1}, \qquad \frac{z_1 - y_1}{x_{11} - y_1} \leq L_1 \leq \frac{z_1 - x_{21}}{x_{11} - x_{21}},$$

$$0 \leq L_2 \leq \frac{x_{11} - z_1}{x_{11} - x_{21}} \qquad (8)$$

For heteroazeotropic mixtures with $z_1 = y_1$, during expansion (P=const, T=const) both liquid phases disappear at the same time, the limit values are L_1=0, L_2=0. For $z_1 = y_1$:

$$0 \leq V \leq 1, \qquad 0 \leq L_1 \leq \frac{y_1 - x_{21}}{x_{11} - x_{21}},$$

$$0 \leq L_2 \leq \frac{x_{11} - y_1}{x_{11} - x_{21}} \qquad (9)$$

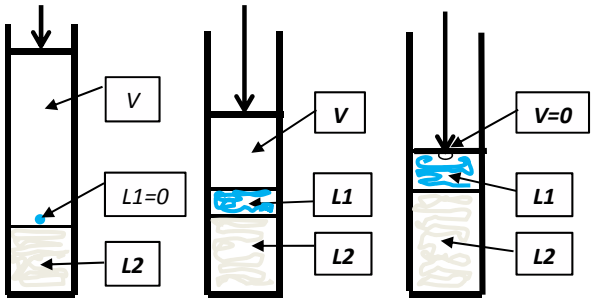


Fig. 3. The change of V, L_1, L_2 at isobaric-isothermal volume change of the binary three-phase mixture of invariant composition ($y_1 \geq z_1 \geq x_{21}$)

For the more volatile component of a zeotropic three-phase mixture (e.g., nitrogen (1) -propane (2)[9]) $y_1 > x_{11} > x_{21}$ (Fig. 2). Provided $x_{11} \geq z_1 \geq x_{21}$, during expansion the more volatile liquid phase 1 disappears, while the vapor phase disappears during compression. Similar to the above, we get:

$$0 \leq V \leq \frac{z_1 - x_{21}}{y_1 - x_{21}}, \qquad 0 \leq L_1 \leq \frac{z_1 - x_{21}}{x_{11} - x_{21}},$$

$$\frac{y_1 - z_1}{y_1 - x_{21}} \leq L_2 \leq \frac{x_{11} - z_1}{x_{11} - x_{21}} \qquad (10)$$

For zeotropic mixtures with $y_1 \geq z_1 \geq x_{11}$, during expansion the more volatile phase 1 disappears, while during compression the vapor phase under the conditions of the three-phase equilibrium does not disappear. In that zeotropic

three-phase mixtures differ from heteroazeotropic ones. For the latter under conditions $x_{11} \geq z_1 \geq x_{21}$, during compression there is a transition from the equilibrium liquid-liquid-vapor (L-L-V) to a liquid-liquid equilibrium (L-L), that is, the vapor phase disappears. For zeotropic mixtures, provided $y_1 \geq z_1 \geq x_{11}$, at compression there is a transition from the L-L-V equilibrium to the more volatile liquid 1-vapor equilibrium (Fig. 2), that is, the less volatile liquid phase 2 disappears. For $y_1 \geq z_1 \geq x_{11}$ the following restrictions are obtained:

$$\frac{z_1 - x_{11}}{y_1 - x_{11}} \leq V \leq \frac{z_1 - x_{21}}{y_1 - x_{21}}, \quad 0 \leq L_1 \leq \frac{y_1 - z_1}{y_1 - x_{11}},$$

$$0 \leq L_2 \leq \frac{z_1 - x_{11}}{x_{11} - x_{21}} \qquad (11)$$

Here are numerical examples of the application of the above restrictions. For water (1) - ethylbenzene system (2) at T = 536.1 K and P=6.50 MPa according to [8] y_1=0.770, x_{11}=0.99675, x_{21}=0.408. With isothermal expansion of the three-phase mixture, the constancy of pressure is maintained due to the evaporation of both liquid phases, but at $y_1 \geq z_1 \geq x_{21}$ (e.g., z_1=0.5) the more volatile water liquid phase will disappear first, and with $x_{11} \geq z_1 \geq y_1$ (e.g., z_1=0.9) the liquid phase 2 will disappear . With z_1=0.5 the mole fractions of phases according to (7) can be in the following limits: $0 \leq V \leq 0.254$; $0 \leq L_1 \leq 0.156$; $0{,}746 \leq L_2 \leq 0.844$. In the above limits, you can arbitrarily set the amount of any phase, others are calculated according to Eqs. (1-3). If you set V = 0.2, then, using Eq. (1), the results are L_1 = 0.033 and L_2 = 0.767.

The same is for z_1=0.9 according to (8): $0 \leq V \leq 0.427$; $0.573 \leq L_1 \leq 0.836$; $0 \leq L_2 \leq 0.164$. For the value V=0.2, and according to Eqs. (1-3), such values are obrained: L_1 = 0.713, L_2 = 0.087.

In accordance with the Gibbs phase rules, three-component and three-phase mixtures are bivariant systems. Therefore, the given temperature and pressure are sufficient information to determine the composition of equilibrium phases. Similar to the two-component mixtures, one can apply the system of Eqs. (1-4). If we assume all K_{1i}, K_{2i} to be known, then we have six nonlinear Eqs. (4) and three Eqs. (2) to determine nine unknown concentrations y_i, x_{1i}, x_{2i}. The system of Eqs. (2, 4) can be solved by the method of elimination of variables:

$$y_1 = \frac{K_{21}\left[K_{23} - K_{22} + \frac{K_{23}(K_{22}-1)}{K_{13}} + \frac{K_{22}(1-K_{23})}{K_{12}}\right]}{\frac{K_{22}(K_{23}-K_{22})}{K_{11}} + \frac{K_{22}(K_{21}-K_{23})}{K_{12}} + \frac{K_{23}(K_{22}-K_{21})}{K_{13}}}$$

$$y_2 = \frac{K_{22}\left[\frac{y_1(K_{21}-K_{23})}{K_{21}} + K_{23} - 1\right]}{K_{23} - K_{22}},$$

$$y_3 = 1 - y_1 - y_2 \qquad (12)$$

Other concentrations are determined by y_1, y_2 by means of Eqs. (2,4). For the three cases: K_{1i}=K_{2i}=1; K_{1i}=1, K_{2i}≠1 and K_{1i}=K_{2i}≠1 there are uncertainties $y_1 = \frac{0}{0}$.

The first case corresponds to the critical point of the higher order, when simultaneously the properties of all three phases become identical and $y_i = x_{1i} = x_{2i}$. The second case corresponds to the critical point of liquid 1 – vapor system in the presence of the second liquid phase (y_i=x_{1i}≠x_{2i}). The third case corresponds to the critical point of solubility of liquid 1-liquid 2 in the presence of the vapor phase (y_i≠x_{1i}=x_{2i}). In the all considered cases, the number of phases is less than three, with the number of unknown concentrations greater than the number of available Eqs.. When using the Formulas (12, 2, 4), it is necessary to make sure that all calculated concentrations belong to the interval [0,1], since either given T and P, or used mathematical models of K_{ij} may not meet the liquid-liquid-vapor equilibrium conditions. This is illustrated by the example of calculating the equilibrium phases of the mixture of butylene (1) - n-butane (2) - water (3) at T = 377.6 K and P=1.757 MPa. These conditions, according to [11], correspond to the liquid-liquid-vapor equilibrium. Let's apply the simplest mathematical models of K_{ij} - the Raoult-Dalton's law for the main components of the liquid phases:

$$K_i = \frac{P_{si}}{P} \qquad (13)$$

and Henry's law for additive components:

$$K_i = \frac{H_{ij}}{P} \qquad (14)$$

where P_{si} is the saturated vapor pressure of the i-th component, H_{ij} is the Henry's constant.

At T=377.6 K the values of the saturated vapor pressure of the components are P_{s1}=1.95 MPa, P_{s2}=1.67 MPa and P_{s1}=0.117 MPa [10]. At T=377.6 K Henry's constants are determined by experimental data [11] for binary mixtures of butylene-water and n-butane-water. They are: for butylene in water H_{13} = 4820 MPa and for n-butane in water H_{23} = 16000 MPa. For water in solution butylene-n-butane we will take H_3 = 8.2 MPa, the average between H_{31} = 10.0 MPa and H_{32} = 6.4 MPa. Table 1 shows the calculated and experimental K_{ij} values and their relative deviations. When substituting the calculated value of K_{ij} in Eqs. (12), the negative value y_1 = – 0.019 is received, which means that the three-phase equilibrium can not be described by the determined K_{ij}.

For the same temperature T = 377.6 K and the higher pressure P = 1.869 MPa, the calculated values Kij by Eqs. (12, 2, 4) ensured the validity that all concentrations belong the interval [0,1] (Table 2).

Table 1

Comparison of calculated and experimental [11] values of distribution coefficients Kij for butylene (1) – n-butane (2) –water (3) system

T=377.6 K , P=1.757 MPa						
	k_{11}	k_{12}	k_{13}	k_{21}	k_{22}	k_{23}
Experimental data	1.023	0.9477	5.380	2739.0	9073.0	0.05490
Calculation	1.110	0.9505	4.67	2680.0	9100.0	0.0666
δk, %	8.50	0.3	–15.2	–2.20	0.30	21.3

Table.2

Comparison of calculated and experimental [11] values of distribution coefficient Kij and the concentrations of the components of three equilibrium phases for butylene (1) – n-butane (2) –water (3) system

T=377.6 K, P=1.869 MPa									
	k_{11}	k_{12}	k_{13}	k_{21}	k_{22}	k_{23}			
Experimental data	1.002	0.9167	4.150	2577.0	8538.0	0.05271			
Calculation	1.040	0.8882	4.387	2579.0	8560.0	0.06342			
δk, %	3.80	-3.1	5.7	0.07	0.27	20.3			
	Y_1	Y_2	Y_3	X_{11}	X_{12}	X_{13}	X_{21}	X_{22}	X_{23}
Experimental data	0.4948	0.4525	0.0527	0.4937	0.4936	0.0127	0.000192	0.000053	0.999755
Calculation	0.4417	0.5179	0.0634	0.4025	0.5831	0.0145	0.000162	0.000060	0.999777
Δx	0.0761	0.0654	0.0107	0.0912	0.0895	0.0018	0.000030	0.000007	0.000022
δx,%	–15.4	14.5	20.3	–18.5	18.1	13.8	–15.4	14.1	0.002

Despite the satisfactory accuracy of the description of five from six values of Kji (only for water δK_{23}=20%), due to the complex structure of error handling, the relative errors of calculating the composition of phases are quite large (15-20%). That is, the calculation based on the laws of Raoult and Henry allows to obtain only the approximate values. To achieve greater accuracy, it is necessary to apply more sofisticated models.

If the overall composition of a ternary three-phase mixture z_i is given and the equilibrium phases composition is known (or calculated), then the mole fractions of phases V, L_1, L_2 can be calculated analytically (instead the solution of the nonlinear system (5)):

$$V=\frac{(z_1-x_{21})(x_{12}-x_{22})-(z_2-x_{22})(x_{11}-x_{21})}{(y_1-x_{21})(x_{12}-x_{22})-(y_2-x_{22})(x_{11}-x_{21})}$$

$$L_1 = \frac{(z_1 - x_{21})(y_2 - x_{22}) - (z_2 - x_{22})(y_1 - x_{21})}{(x_{11} - x_{21})(y_2 - x_{22}) - (x_{12} - x_{22})(y_1 - x_{21})}$$

$$L_2 = 1 - V - L_1 \qquad (15)$$

In Eqs. (15) the necessary boundary transitions are executed:
for $z_i = y_i$ and $x_{1i} \neq x_{2i}$ $V=1$, $L_1 = L_2 = 0$,
for $z_i = x_{1i}$ and $x_{1i} \neq x_{2i}$ $V = L_2 = 0$, $L_1 = 1$
and for $z_i = x_{2i}$ and $x_{1i} \neq x_{2i}$ $V = L_1 = 0$, $L_2 = 1$.

For $y_i = x_{1i} = x_{2i}$; $x_{1i} = x_{2i}$; $y_i = x_{2i}$ and $y_i = x_1$ there are uncertainties, the causes of which are analogous to those discussed for Eqs. (12). The values V, L_1, L_2 calculated using Eqs. (15) may not belong to the interval [0,1] if the given z_i does not provide the possibility of coexistence of the three phases.

In Fig. 4 for the fixed T and P the equilibrium composition of vapor V and two liquid phases L1 and L2 are shown by the points, and 7 regions of overall composition of mixtures corresponding to three-, two- and single-phase states are indicated.

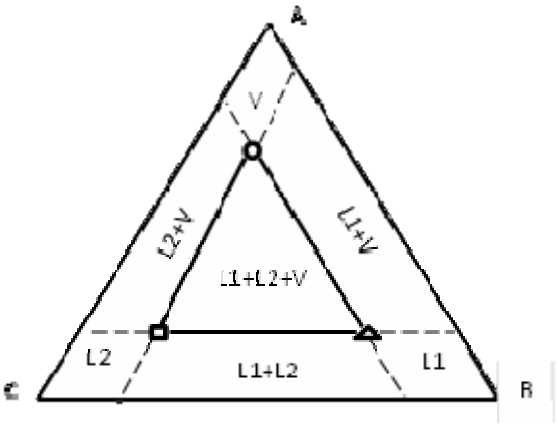


Fig. 4. Areas of phase states that are possible during isobaric-isothermal change of the total composition of a ternary mixture A + B + C.

The equilibrium of liquid-liquid-vapor L1 + L2 + V corresponds to the case $0 \leq V \leq 1$, $0 \leq L_1 \leq 1$, $0 \leq L_2 \leq 1$. For the two-phase equilibrium of the liquid L1-liquid L2: $V < 0$, $0 \leq L_1 \leq 1$, $0 \leq L_2 \leq 1$. For the two-phase equilibrium of the liquid 1-vapor:
$0 \leq V \leq 1$, $0 \leq L_1 \leq 1$, $L_2 < 0$. For the two-phase equilibrium of the liquid 2-vapor: $0 \leq V \leq 1$, $L_1 < 0$, $0 \leq L_2 \leq 1$. For regions of single-phase states: for vapor $V > 1$, for liquid 1 $L_1 > 1$, for liquid 2 $L_2 > 1$.

For an example, considered above at T = 377.6 K, P = 1.869 MPa, the butylene–n-butane-water mixture having a composition of $\{z_1 = 0.40; z_2 = 0.40, z_3 = 0.20\}$ is in the two-phase state of liquid 1- liquid 2 ($V = -0.0026$), with $\{z_1 = 0.40; z_2 = 0.37, z_3 = 0.23\}$ is in the three-phase state ($V = 0.708$, $L_1 = 0.100$, $L_2 = 0.192$), with $\{z_1 = 0.40; z_2 = 0{,}36, z_3 = 0{,}24\}$ is in the two-phase state, the aqueous liquid 2-vapor ($L_1 = -0{,}137$). Experimental data of the phase composition values (Table 2) were used for calculation by Eqs. (15).

6. Discussion

The application of the general algorithm for solving Eqs. (1-5) to binary mixtures usually results in ambiguity of the calculated values of L_1, L_2, V. Therefore, it is expedient to use the restrictions imposed by Formulas (7-11) for this case and add the input information to the valid value of one of the unknowns (V or C). For ternary mixtures for indicative calculations, or as a first approximation, Formulas (12-15) can be used both for determining the composition of coexisting equilibrium phases and for determining the mole fraction of phases. To do this, numerical values of the corresponding Henry's constants are needed.

7. Conclusions

The considered features of binary and ternary mixtures should be considered in the algorithm for calculating the three-phase equilibrium of multicomponent mixtures.

References

[1] Sydorov Yu.Sh., Vlyazlo R.Y., Novikov V.P. (2008) *Protsesy i aparaty mikrobiolohichnoyi ta farmatsevtychnoyi promyslovosti* [Processes and apparatuses of microbiological and pharmaceutical industries]. Lviv, Intelekt-Zakhid Publ., 736 p. (in Ukrainian).

[2] Doran P. M. (2013) *Bioprocess engineering principles*. Oxford, Academic press, 919 p.

[3] Soetaert W., Vandamme E. J. (Eds.). (2010). *Industrial biotechnology: sustainable growth and economic success*. John Wiley & Sons, 499 p.

[4] Walas S.M. (1985) *Phase Equilibria in Chemical Engineering*. Boston, Butterworth Publ., 664 p.

[5] Reddy P.S., Rani K.Y. (2012) A Simple Algorithm for Vapor-Liquid-Liquid Equilibrium

Computation. *Industrial & engineering chemistry research*, vol.51, no. 32, pp.10719-10730. doi: 10.1021/ie 2022064.

[6] Wyczesany A. (2012) Calculation of Vapour-Liquid-Liquid Equilibria in Quaternary Systems. *Chemical and Process Engineering*, vol. 33, no 3, pp.463-477. doi: 10.2478/vl 10176-012-0039-5.

[7] Cismondi M., Michelsen M.L. (2007) Global phase equilibrium calculations: Critical lines, critical end points and liquid-liquid-vapour equilibrium in binary mixtures. *The Journal of supercritical fluids*, vol. 39, no. 3, pp. 287-295.

[8] Heidman J.L., Tsonopoulos C., Brady C.J., Wilson G.M. (1985) High-temperature mutual solubilities of hydrocarbons and water . *AIChE Journal*, vol. 31, no. 3, pp. 376-384.

[9] Llave F.M., Luks K.D., Kohn J.P. (1985) Three-Phase Liquid-Liquid-Vapor Equilibria in the Binary Systems Nitrogen+Ethane and Nitrogen+Propane. *Journal of Chemical & Engineering Data*, vol. 30, no. 4, pp. 435-438. doi: 10.21/je00042a019.

[10] Vargaftik N.B. (1972) *Spravochnik po teplofizicheskim svoystvam gazov i zhidkostey* [Handbook of thermophysical properties of gases and liquids]. Moscow, Nedra Publ., 720 p. (in Russian).

[11] Wehe A.H., Mc Ketta J.J.(1961) Butene - n-butane-water system in two- and three-phase regions. *Journal of Chemical and Engineering Data*, vol. 6, no. 2, pp. 167-176.

Received 12 January 2018

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Особливості розрахунку для процесів екстракції матеріального балансу трьохфазних сумішей

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Мета: Вдосконалення алгоритму розрахунку рівноваги рідина-рідина-пара для бінарних та трьохкомпонентних сумішей (для процесів екстракції)**. Методи:** Аналіз фазових діаграм, моделювання відсікання частини рівноважної фази, алгебраїчні перетворення системи рівнянь задачі одноразового випаровування трьохфазної суміші заданого складу**. Результати:** Для двох типів фазових діаграм двокомпонентних сумішей з обмеженою розчинністю компонентів в рідкій фазі отримані обмеження на можливі значення молярних часток парової та двох рідких фаз за умов рівноваги рідина-рідина-пара для суміші заданого загального складу. Для трьохкомпонентних сумішей отримані аналітичні вирази для розрахунку складів трьох фаз за заданими двома наборами коефіцієнтів розподілу. Отримані формули для розрахунку молярних часток парової та двох рідких фаз за заданим загальним складом суміші. Наведені формули застосовані для розрахунку трьохфазної рівноваги суміші бутилен-н-бутан-вода на підставі законів Рауля та Генрі. **Обговорення**: Для трьохкомпонентних сумішей для орієнтовних розрахунків можна застосувати отримані формули як для визначення складів співіснуючих рівноважних фаз, так і для визначення молярних часток фаз. Для бінарних сумішей доцільно доповнити вхідну інформацію задачі одноразового випаровування суміші заданого складу припустимим значенням молярної частки парової фази.

Ключові слова: біотехнологія; екстракція; коефіцієнт розподілу; матеріальний баланс; рівновага рідина-рідина-пара; розрахунок; суміш.

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Особенности расчета для процессов экстракции материального баланса трёхфазных смесей

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Цель: Совершенствование алгоритма расчета равновесия жидкость-жидкость-пар для бинарных и трёхкомпонентных смесей (для процессов экстракции). **Методы:** Анализ фазовых диаграмм, моделирование отсечения части равновесной фазы, алгебраические преобразования системы уравнений задачи однократного испарения трёхфазной смеси заданного состава. **Результаты:** Для двух типов фазовых диаграмм двухкомпонентных смесей с ограниченной растворимостью компонентов в жидкой фазе получены ограничения на возможные значения молярных долей паровой и двух жидких фаз в условиях равновесия жидкость-жидкость-пар для смеси заданного общего состава. Для трёхкомпонентных смесей получены аналитические выражения для расчета составов трёх фаз по заданным двумя наборами коэффициентам распределения. Получены формулы для расчета молярных долей паровой и двух жидких фаз по заданному общему составу смеси. Приведенные формулы применены для расчета трёхфазного равновесия смеси бутилен-н-бутан-вода на основании законов Рауля и Генри. **Обсуждение:** Для трехкомпонентных смесей для ориентировочных расчетов можно применить полученные формулы как для определения составов сосуществующих равновесных фаз, так и для определения молярных долей фаз. Для бинарных смесей целесообразно дополнить входную информацию задачи однократного испарения смеси заданного состава допустимым значением молярной доли паровой фазы.

Ключевые слова: биотехнология; коэффициент распределения; материальный баланс; равновесие жидкость-жидкость-пар; расчет; смесь; экстракция.

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